1. GENERAL INFORMATION

1.1 NUMBER 64667-33-0

1.2 CHEMICAL NAME Methyl 4,6,6,6-tetrachloro-3,3-dimethylhexanoate

1.3 EXPOSURE (CLOSED SYSTEM)

1.3.1. PROCESS DESCRIPTION

DVEster Step II is produced at the B-34 facility in the FMC Baltimore Plant.

DVEster Step II product (FMC 30099) is produced by the reaction between Step I product (FMC 30098) and carbon tetrachloride (CCl_4) in the presence of a catalyst, benzoyl peroxide (BPO). See Figure 1 below.

Carbon tetrachloride is atmospherically stripped out of the reaction mass. Then a vacuum strip is performed to remove residual carbon tetrachloride and reaction by-products. The Step II product is then transferred to storage.

Step II product (FMC 30099) and sodium methylate are reacted to produce DVester (FMC 39338) in a batch reaction. Figure 2 shows the Step III reaction system. An excess sodium methylate/heptane slurry is mixed in T-310 and then fed to the reactor (R-301). After the slurry is heated, the reaction begins when Step II product is fed to the reactor.

The Step II product is converted to DVester through a series of irreversible dechlorination reactions. Two chlorines must be removed from the Step II before it becomes DVester. A total of 97-98% of the Step II is converted to DVester with the remaining percentage having only one chlorine removed (i.e, no longer existing as Step II material). The entire system is closed.

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FIGURE 1
Step II Process Description

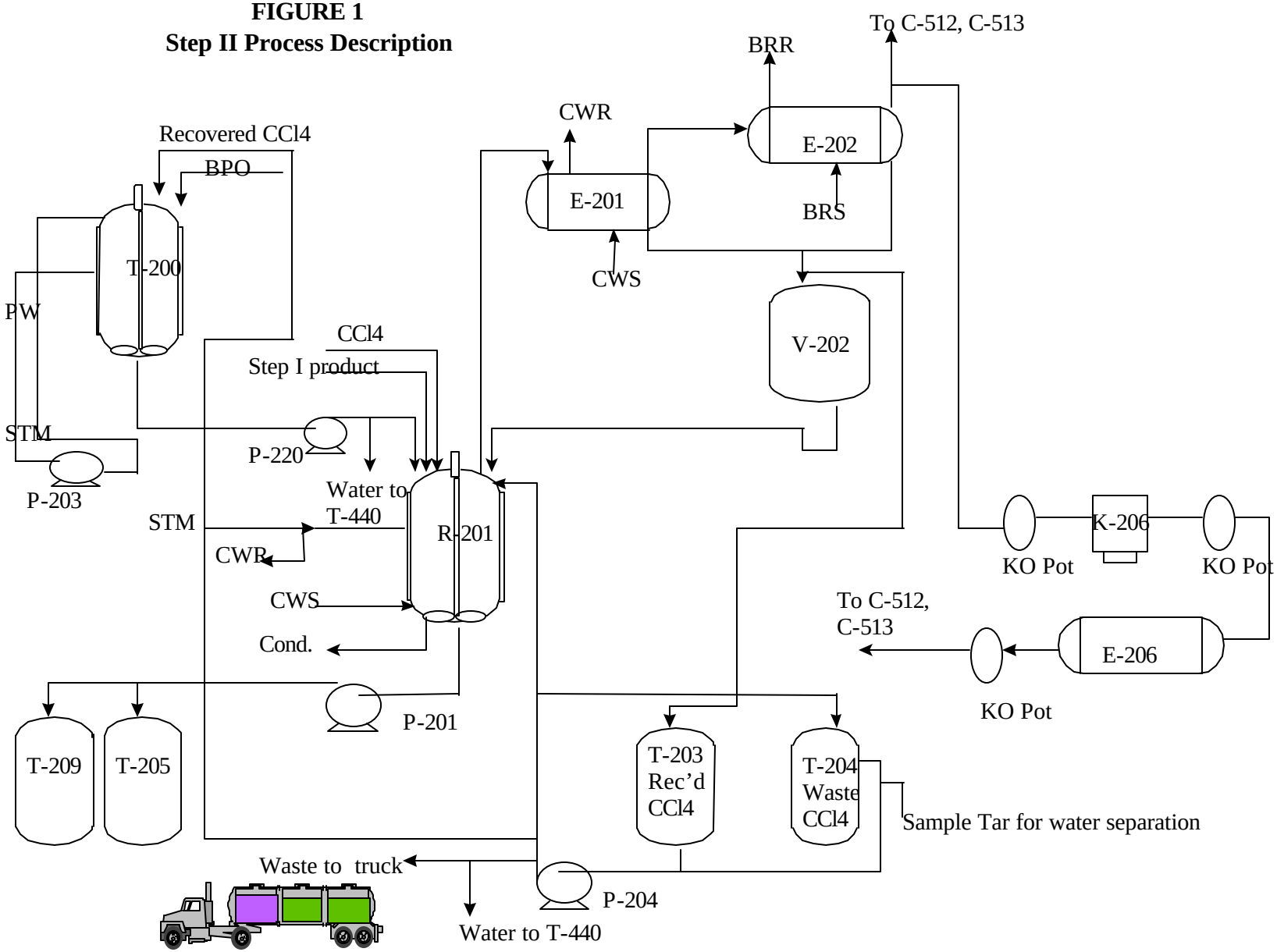
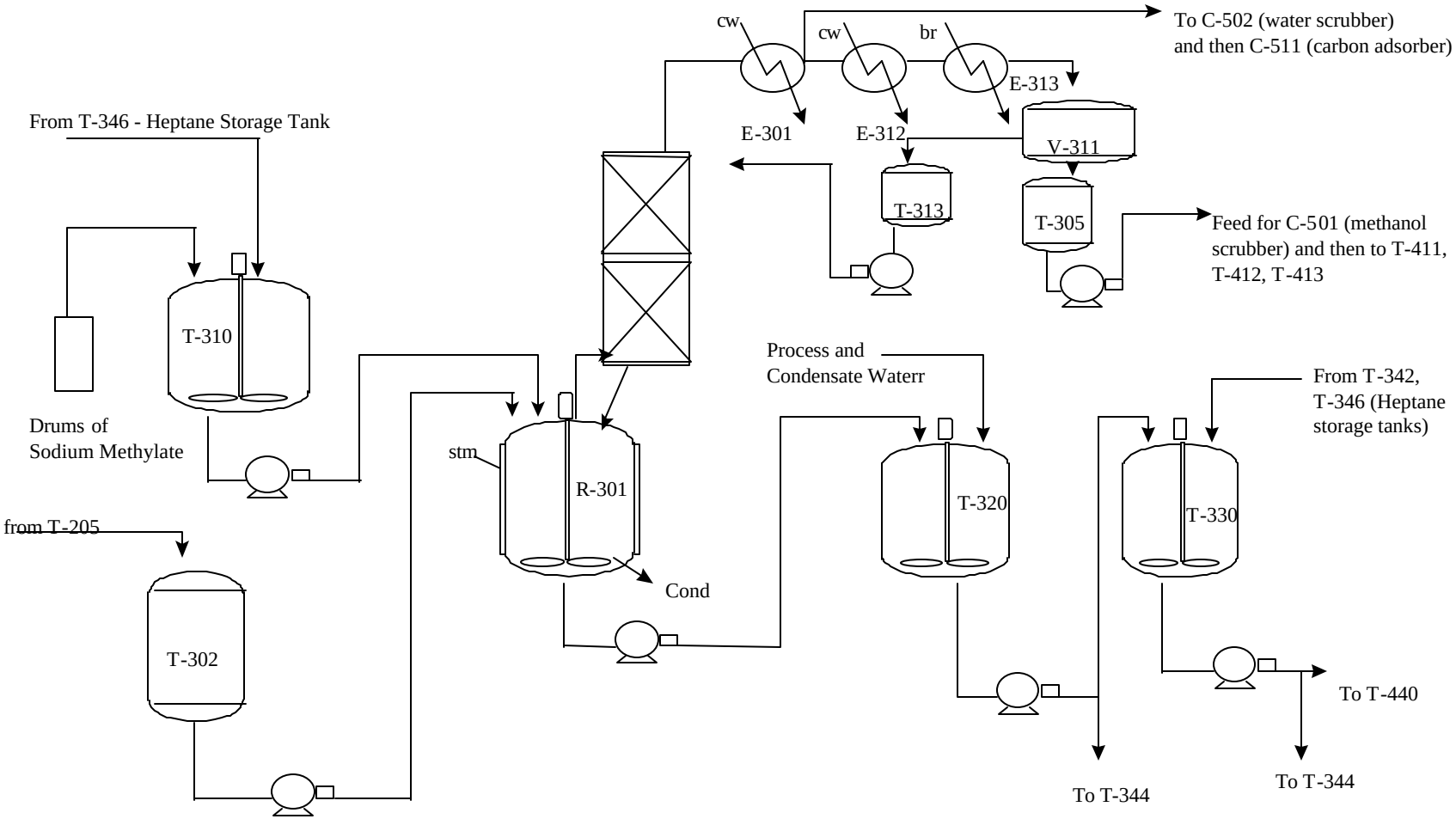


FIGURE 2
Step III Reaction and Wash System



T-205 Step II Product Storage Tank	T-310 SodiumMethylate Slurry Charge Tank	T-301 Step III Reactor Column	E-301 Step III Reactor Condenser	E-313 Step III Reactor After Condenser	V-311 Step III Reactor Decanter	T-320 Step III Wash Tank	T-330 Step III Extraction Tank	T-440 Waste Water Storag Tank
	T-302 Step III Product Feed Tank	R-301 Step III Reactor	E-312 Step III Chiller	T-313 Reflux Surge Tank	T-305 Waste Methanol Surge Tank	T-344 Heptane Stripper Feed Tank	T-411, 412, 413 Waste Methanol Storage Tanks	

1.3.2. MONITORING DATA

Wastewater monitoring - Wastewater samples are taken before every pump down to the south plant carbon beds. The limit for Step II in the water is 25 ppm. In 2001, our average concentration of Step II in this wastewater stream was 14.8 ppm.

IH Data – IH monitoring conducted in 1985 and 1988 indicated non detectable levels of Step II product in air. The limit of detection for the monitoring at that time was 0.1 mg.

1.3.3. PRESENCE IN DISTRIBUTED PRODUCT

No Dvester Step II is present in the Dvester Finished Goods products.

1.3.4 TRANSPORT DATA

Step II DVester is not transported.

1.3.5 PRESENCE IN END USE PRODUCTS

Confidential Statements of Formula - DVEster Step II is not included on any Confidential Statement of Formula for the technical materials produced in Baltimore using DVEster Step III Finished Goods as a raw material.

Literature Search - Results from a Chemical Abstracts On-line Database literature search indicate that DVEster Step II is not present in other end-products.

2. PHYSICAL AND CHEMICAL DATA

2.1 MELTING POINT

No data available.

2.2 BOILING POINT

2.2.1. SOURCE #1

Test Substance:	Methyl 4,6,6,6-tetrachloro-3,3-dimethylhexanoate
Method:	Unknown
GLP:	No
Year:	1978
Results:	110 - 114 ° C @ 93.3 Kpa (0.7 mm Hg)
Data Quality:	4e

References: "Permethrin Compendium", M. Fishman, November 17, 1980

2.2.2 SOURCE #2

Test Substance: Methyl 4,6,6,6-tetrachloro-3,3-dimethylhexanoate

Method: Vacuum distillation

GLP: No

Year: 1999

Results: 101-103 ° C @ 0.1 mm Hg

Data Quality: 4e

References: Synthetic Communications 29(10), 1653-1659 (1999)

2.3 VAPOR PRESSURE

Test Substance: Methyl 4,6,6,6-tetrachloro-3,3-dimethylhexanoate, 100% pure

Method: Unknown

GLP: No

Year: Unknown

Results: 0.6 mm Hg @ 100^{o}C

Data Quality: 4e

References: FMC MSDS

2.4 PARTITION COEFFICIENT No data available.

2.5 WATER SOLUBILITY

Test Substance:	Methyl 4,6,6,6-tetrachloro-3,3-dimethylhexanoate
Method:	Unknown
GLP:	No
Year:	Unknown
Results:	Insoluble
Data Quality:	4e
References:	FMC MSDS

3 ENVIRONMENTAL FATE AND PATHWAY

3.1 PHOTODEGRADATION

Test Substance:	Methyl 4,6,6,6-tetrachloro-3,3-dimethylhexanoate
Method:	Estimated by the AOP program (v. 1.90) which estimates rate constants and half-lives of atmospheric reactions of organic compounds with hydroxyl radicals and ozone in the atmosphere.
GLP:	No
Year:	2000
Results:	For reaction with hydroxyl radicals, the predicted half-life is 5.2 days with a rate constant of 2.04×10^{-12} cm^3/molecule-sec.
Remarks:	The photodegradation calculation by an acceptable method is assigned a reliability code of 2f.
References:	AOPWIN version 1.90, Syracuse Research Corporation, Syracuse, NY

3.2 STABILITY IN WATER (HYDROLYSIS)

Test Substance: Methyl 4,6,6,6-tetrachloro-3,3-dimethylhexanoate

Method: Estimated by HYDROWIN program (v. 1.67)

GLP: No

Year: 2000

Results: The predicted half-life is 5.4 years at pH 8 and 54 years at pH 7.

Remarks: The hydrolysis calculation by an acceptable method is assigned a reliability code of 2f.

References: HYDROWIN version 1.67, Syracuse Research Corporation, Syracuse, NY

3.3 TRANSPORT/DISTRIBUTION (FUGACITY MODEL)

Test Substance: Methyl 4,6,6,6-tetrachloro-3,3-dimethylhexanoate
Method: Estimated by EPI Suite program (v. 3.05)

GLP: No

Year: 002

Results: Distribution using Level III Fugacity model

	Concentration (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.67	125	1000
Water	9.71	3.6e+003	1000
Soil	72	3.6e+003	1000
Sediment	17.6	1.44e+003	0

Remarks: The fugacity calculation by an acceptable method is assigned a reliability code of 2f.

References: EPI Suite version 3.05, Syracuse Research Corporation, Syracuse NY

3.4 BIODEGRADATION No data available.

4 ECOTOXICOLOGY

4.1 ACUTE TOXICITY TO FISH

Test Substance:	Methyl 4,6,6,6-tetrachloro-3,3-dimethylhexanoate
Method:	EPA, 1975, Methods for Acute Toxicity Tests with Fish, Macroinvertebrates, and Amphibians. Ecological Research Series EPA-660/3-75-009. 61 p. Test was conducted under static condition in 19 L uncovered jars which contained 15 L of natural, filtered (5 micrometers) sea water. Salinity was 17 parts per thousand. Temperature was maintained at 20 °C +/- 1. Initial pH was 8 +/- 0.5 for all test concentrations and controls. The sheepshead minnows measured 7 – 12 mm in standard length. Mortality was <3% during a 7-day acclimation period. The fish appeared to be in excellent condition at initiation of the test. Each test jar contained 10 fish. There was no aeration. Based on preliminary tests, sheepshead minnows were exposed to five concentrations of the test material. Test material was dissolved in reagent grade acetone and pipetted into sea water in the appropriate test containers to obtain the desired concentrations. A vehicle control was run with a volume of acetone equal to that added to the highest test concentration.
Species:	Sheepshead minnow (*Cyprinodon variegates)*
Test Concentration (nominal):	Control (0), 1.8, 3.2, 5.6, 7.5 and 10 ppm
Exposure Period:	96 hours
Analytical Monitoring:	No
GLP:	No
Year:	1976
Results:	The estimated 96-hour LC50 for sheepshead minnows in static, unaerated sea water was greater than 3.2 ppm but less than 5.6 ppm. Dissolved oxygen remained >65% of saturation in all test concentrations and controls for the duration of the test. The final pH was 8 +/- 0.5 for all test concentrations and controls.
Conclusion:	The 96-hour LC_{50} was between 3.2 and 5.6 ppm.

Data Quality:	2d
References:	Acute Toxicity of four compounds to Sheepshead Minnows (*Cyprinodon variegates)*, EG&G, Bionomics, FMC Study Number ACT 015.11-03, April 1976.

4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

No data available.

4.3 TOXICITY TO AQUATIC PLANTS

No data available.

5 TOXICITY

5.1 ACUTE TOXICITY

5.1.1 ORAL

Test Substance:	Methyl 4,6,6,6-tetrachloro-3,3-dimethylhexanoate, purity > 97%
Method:	US EPA Pesticide Assessment Guidelines; Subdivision F, Hazard Evaluation: Human and Domestic Animals, November, 1982; 81-2 Acute Oral Toxicity Study. Ten rats (5 male and 5 female) were orally dosed with undiluted test material at a dosage of 5000 mg/kg. Observations for toxicity were conducted at 0.5, 1, 2, 3, 4 and 6 hours post-dosing and twice daily thereafter for thirteen days. On day 14, observations were only performed once. Body weights were recorded on days 0, 7 and 14 of the study. Gross necropsy was performed on all animals.
Species/strain:	Sprague-Dawley
Sex:	Male and Female
No. Animals/Group:	5/sex/ group
Dose:	5000 mg/kg
Post-dosing observation period:	14 days
GLP:	Yes

Year:	1984
Results:	There were no deaths. Predominant clinical signs included abdominogenital staining, diarrhea, exophthalmos, lacrimation, decreased locomotion, nasal discharge and oral discharge. All signs subsided by day eight of the study. All surviving animals gained weight by day 14 of the study. There were no gross lesions in any animal at gross necropsy.
Conclusion:	The test material is classified as practically non-toxic with a LD50 greater than 5000 mg/kg for both male and female rats.
Data Quality:	1
References:	Acute Oral Toxicity of FMC 30099 Technical in Rats, FMC Study Number A1984-1459, July 29, 1985.

5.1.2 DERMAL

Test Substance:	Methyl 4,6,6,6-tetrachloro-3,3-dimethylhexanoate, purity >97%
Method:	The test substance was applied topically to the backs of 10 rabbits, 5 rabbits per dosage, under occluded conditions for 24 hours. Observations for toxicity were conducted daily, irritation was evaluated after 1, 2, 3, 4, 7 and 14 days.
Species/strain:	New Zealand White Rabbits
No. Animals:	5 animals/group
Dose:	423 mg/kg and 28.2 mg/kg
Vehicle:	None
Exposure Period:	24 hours
Post-exposure observations:	Observations for toxicity: daily Observations for irritation: 1, 2, 3, 4 and 7 days
GLP:	Yes
Year:	1985

Results:	There were no deaths. All rabbits remained healthy throughout the study. No treatment-related weight change was observed. Slight erythema and desquamation were noted sporadically. No gross lesions were observed at necropsy.
Conclusion:	The test substance was practically non-toxic and minimally irritating.
Data Quality:	2c
References:	Preliminary Dermal Toxicity/Irritation of FMC 30098 Technical in Rabbits, FMC Toxicology Laboratory, FMC Study A84-1419, April 25, 1985.

5.1.3 INHALATION

Test Substance:	Methyl 4,6,6,6-tetrachloro-3,3-dimethylhexanoate, purity > 97%
Method:	Five male and five female rats were exposed to the vapor of the test material for six hours at a nominal concentration of 5.5 ppm in a dynamically-operated, whole-body inhalation exposure chamber. Observations for toxicity and mortality were performed frequently during the exposure, upon removal from the chamber, at one hour post-exposure, and daily thereafter for fourteen days. Individual body weights were recorded immediately prior to exposure (day 0) and on days 7 and 14. On day 14, all animals were sacrificed and complete gross necropsy examinations were performed.
Species/strain:	Sprague-Dawley
No. Animals:	5/sex/group
Dose:	5.5 ppm
Vehicle:	undiluted
Exposure Period:	6 hours
Post-exposure observation period:	14 days
GLP:	Yes
Year:	1987
Results:	There were no deaths during the study. Clinical signs noted among test rats during the first hour of exposure included irregular breathing patterns and one rat had red periocular fur around the left eye at

removal. One of the control rats had perinasal fur upon removal from the chamber. Body weight changes occurred in the usual manner. No internal gross lesions were noted in any animal at necropsy.

The airborne concentration which represented essentially saturated vapors of the test substance was low and produced only a transient toxic response, suggestive of irritation during expose.

Conclusion: The inhalation LC_{50} was greater than 5.5 ppm.

Data Quality: 2c

References: FMC 39008 Technical, Acute Inhalation Toxicity Screen in Rats, FMC Toxicology Laboratory, FMC Study A85-1660, July 10, 1987.

5.2 REPEATED DOSE TOXICITY No data available.

5.3 GENETIC TOXICITY IN VITRO AND IN VIVO

5.3.1 GENE MUTATION

Test Substance: Methyl 4,6,6,6-tetrachloro-3,3-dimethylhexanoate, Purity > 97%

Method: *Salmonella typhimurium*/Mammalian Microsome Plate Incorporation Mutagenicity Assay (Ames Test). The test was conducted using *Salmonella typhimurium* tester strains TA1535, TA1537, TA1538, TA98, TA100 with and without metabolic activation by rat liver microsomes, S9, using the standard protocol. The positive controls included sodium azide, 9-aminoacridine, 2-nitrofluorene and 2-anthramine. The negative control was the solvent DMSO. The criteria for positive results were derived from Principles of Genetic Toxicology (1980).

The test article was solubilized in DMSO and serially diluted immediately before its use in the mutagenicity assay. Five doses of the test material were plated with all five tester strains with and without metabolic activation. All solvent controls and test article doses were plated in triplicate.

Type: In vitro mutagenicity in bacteria

System of Testing: *Salmonella typhimurium* TA1535, TA1537, TA1538, TA98, TA100 with and without metabolic activation by Aroclor induced rat liver microsomes, S9.

Concentration: 10 to 10,000 ug/plate

Metabolic Activation: S9

GLP:	Yes
Year:	1986
Results:	The test material did not cause a positive response in any of the five tester strains with or without metabolic activation.
Data Quality:	1a
References:	Salmonella/Mammalian-Microsome Plate Incoproration Mutagenicity Assy (Ames Test), FMC Genetic Toxicology Laboratory, FMC Study Number A84-1449, April 6, 1986.
	Brusick, D. Principles of Genetic Toxicology. P. 195, Plenum Press, New York, 1980.

5.3.2 CHROMOSOMAL ABERRATION No data available.

5.4 REPRODUCTIVE TOXICITY No data available.

5.5 DEVELOPMENTAL TOXICITY/TERATOGENICITY No data available.

CRITERIA FOR RELIABILITY CODES

(Adapted from Klimisch et al 1997)

Code of Reliability	Category or reliability
1	**Reliable without restriction**
1a	GLP guideline study (OECD, EC, EPA, FDA, etc.)
1b	Comparable to guideline study
1c	Test procedure in accordance with generally accepted scientific standards and described in sufficient detail
2	**Reliable with restrictions**
2a	Guideline study without detailed documentation
2b	Guideline study with acceptable restrictions
2c	Comparable to guideline study with acceptable restrictions
2d	Test procedure in accordance with national standard methods with acceptable restrictions
2e	Study well documented, meets generally accepted scientific principles, acceptable for assessment
2f	Accepted calculation method
2g	Data from handbook or collection of data
3	**Not reliable**
3a	Documentation insufficient for assessment
3b	Significant methodological deficiencies
3c	Unsuitable test system
4	**Not assignable**
4a	Abstract
4b	Secondary literature
4c	Original reference not yet available
4d	Original reference not yet translated
4e	Documentation insufficient for assessment